PROGRAM ORFFE

Description of input control cards.

(1) Title Card (A72)
Any 72 Hollerith characters

(2) Control Card (18I4)

col.

1- 3 INCD = 0 Input of parameters etc. from file ORFFE.DAT

= 1 all inputs from cards

5- 8 IPM = 1 Variance-covariance matrix read from ORFFE.DAT

= 0 No parameter errors used

= -1 Standard errors (without covariances) read from cards

9-12 IAM = 0 Cell parameter errors are not used

= 1 Cell parameter errors to be read in the form of standard errors

= 2 Cell parameter errors to be read in the form of a variance-covariance matrix

13-16 NS The number of symmetry cards to be read (max. 48)

17-20 NA The number of atoms whose parameters are to be read. Irrelevant if INCD = 0.

21-24 ITF The temperature factor indicators. Irrelevant if INCD =0.

= 0 Thermal parameters are not read.

= 1 Positional and isotropic thermal parameters will be read.

= 2 Positional and anisotropic thermal parameters will be read.

Note: if ITC(I) is non-zero for an individual atom (see below), it overrides ITF.

25-28 IJANA = 0 ORFFE.DAT created from ANVLS

= 1 ORFFE.DAT created from JANA5

(3) Atomic parameters -- omit if INCD = 0. Otherwise 1, 2 or 4 cards are included for each of NA atoms. Cards from ANVLS may be used.

(a) Position card (A6,21X,3F9.6)

col.

1- 6 Any 6 Hollerith characters identifying atom I.

7-27 blank (these columns will be ignored by program)

28-36 X \
37-45 Y > fractional coordinates of atom I
45-54 Z /

(b) Temperature factor card (6F9.6,9X,2I3)

col.

1- 9 B(ISO) OR B(11)
10-18 B(22)
19-27 B(33)
28-36 B(12)
37-45 B(13)
46-54 B(23)

55-63 blank

64-66 ITC(I) temperature factor indicator for atom I.

= 0 temperature factor as specified by ITF

= 1 isotropic temperature factors

= 2 anisotropic temperature

67-69 IGM(I) GAMMA tensor indicator

= 0 no GAMMA tensor for this atom

= 1 GAMMA tensor follows this card

Note: cards (c) and (d) are for the GAMMA tensor -- FORMAT(5F14.10). Omit if IGM(I)=0 or if ITF=0.

(4) Standard errors of atomic parameters. Omit if INCD = 0 or IPM = 0. Otherwise, the cards included are analogous to the atomic parameters cards.

(a) (27X,3F9.6)

COL. 1-27 BLANK

28-36 \
37-45 > STANDARD ERROR OF X,Y AND Z
46-54 /

(b) (6F9.6)

COL. 1- 9 Standard errors of B(ISO) OR B(11)

```
           10-18       "      "     " B(22)
           19-27       "      "     " B(33)
           28-36       "      "     " B(12)
           37-45       "      "     " B(13)
           46-54       "      "     " B(23)
```

Cards (c) and (d) contains standard errors of the GAMMA tensor -- FORMAT(5F14.10). Omit if IGM(I) = 0 or ITF = 0.

(5) LATTICE PARAMETERS (6F9.6)

```
      COL.   1- 9   A
            10-18   B
            19-27   C
            28-36   COS(ALPHA)
            37-45   COS(BETA)
            46-54   COS(GAMMA)
```

(6) Standard errors of lattice parameters -- include if IAM = 1.

```
      COL.   1- 9   Standard errors of A
            10-18      "       "    "  B
            19-27      "       "    "  C
            28-36      "       "    "  COS(ALPHA)
            37-45      "       "    "  COS(BETA)
            46-54      "       "    "  COS(GAMMA)
```

(7) Variance-covariance matrix for lattice parameters. Used only if IAM = 2.

```
   (a) COL.  1- 9   Variance of A
             10-18   Covariance of A and B
             19-27   Covariance of A and C
             28-36   Covariance of A and COS(ALPHA)
             37-45   Covariance of A and COS(BETA)
             46-54   Covariance of A and COS(GAMMA)
             55-63   Variance of B
             64-72   Covariance of B and C

   (b) COL.  1- 9   Covariance of B and COS(ALPHA)
             10-18   Covariance of B and COS(BETA)
             19-27   Covariance of B and COS(GAMMA)
             28-36   Variance of C
             37-45   Covariance of C and COS(ALPHA)
             46-54   Covariance of C and COS(BETA)
             55-63   Covariance of C and COS(GAMMA)
             64-72   Variance of COS(ALPHA)

   (c) COL.  1- 9   Covariance of COS(ALPHA) and COS(BETA)
             10-18   Covariance of COS(ALPHA) and COS(GAMMA)
             19-27   Variance of COS(BETA)
             28-36   Covariance of COS(BETA) and COS(GAMMA)
             37-45   Variance of COS(GAMMA)
```

(8) SYMMETRY INFORMATION -- NS cards each of which describes one symmetry transformation. If all distances are to be computed, read in all equivalent positions including the basic position X,Y,Z and those related by center of symmetry and by unit cell centering. FORAMT(3(F15.10,3F3.0))

The transformed coordinates are in the form:

```
X(NEW) = T(X) + M(XX)*X + M(XY)*Y + M(XZ)*Z
Y(NEW) = T(Y) + M(YX)*X + M(YY)*Y + M(YZ)*Z
Z(NEW) = T(Z) + M(YX)*X + M(ZY)*Y + M(ZZ)*Z
```

| COL. | |
|---|---|
| 1-15 | T(X) |
| 16-18 | M(XX) |
| 19-21 | M(XY) |
| 22-24 | M(XZ) |
| 25-39 | T(Y) |
| 40-42 | M(YX) |
| 43-45 | M(YY) |
| 46-48 | M(YZ) |
| 49-63 | T(Z) |
| 64-66 | M(ZX) |
| 67-69 | M(ZY) |
| 70-72 | M(ZZ) |

(9) Instruction cards are as described below. Include as many as needed to define the quantities to be computed.

(10) Termination card (I5)

col. 1-5 = 0 terminate job

= -1 start new job reading new title card, etc.

**********
Instruction Input:

Each function to be computed is specified by a sequence of integers (IN), which are read from one or more instruction cards. The first integer in this sequence, IN(1), defines the type of function to be computed, and the interpretation of the remaining instruction integers will be different for different types of functions. Details of the instruction integers for each type of function are given below.

Each instruction card is read with format(14I5). Of the 14 integers on this card, only the first 13 are considered to be part of the instruction. If a function requires more than 13 integers to define it, then punching a "1" in column 70 indicates that the instruction is continues on the next card.

**********
Atom Description

In the instructions described below, each atom I is designated by two integers, AI and SI, defined as follows:

AI is the number of the atom in the parameter list. The unit cell origin may by designated by setting AI at "0".

SI is a five-digit number, the two low-order digits of which specify the number of the symmetry operation (symmetry card number) to be applied. Zero may be used to refer to the reference asymmetric unit transformation X,Y,Z even though this identity transformation should be present somewhere in the symmetry card.

The three high-order digits of SI specify unit cell translation along A,B,C, respectively, with 5 added to each digit. Thus 655 implies a translation of one unit cell in the A-direction. An exception is that the reference cell may be referred to as 000 or 555.

Note: an atom in the basic asymmetric unit may be specified by leaving SI blank.

**********
Instruction Cards (14I5):

(1) #001 Distance between atoms 1 and 2

| col. | 5 | 10 | 15 | 20 | 25 |
|---|---|---|---|---|---|
| | 1 | A1 | S1 | A2 | S2 |

#101 All distances less than MAX/100 between origin atoms with numbers A1 to A2 and target atoms A3 to A4.

| col. | 5 | 10 | 15 | 20 | 25 | 30 |
|---|---|---|---|---|---|---|
| | 101 | A1 | A2 | A3 | A4 | MAX |

#201 Same as #101 but also computes angles with origin atoms as vertices. If MAX is large, then the number of angles will also be larger.

```
col.  5   10   15   20   25   30
    201   A1   A2   A3   A4   MAX
```

(2) #002 Angle defined by three atoms. Atom 2 is vertex.

```
col.  5   10   15   20   25   30   35
    002   A1   S1   A2   S2   A3   S3
```

(3) #003 Angle between normals to planes defined by atoms 1, 2 and 3, and atoms 4, 5 and 6, respectively. If right-hand fingers are curved so that they can pass successively through atoms 1, 2 and 3 then the thumb is in direction of normal. Sign of angle will be positive if this normal makes an acute angle with vector from atoms 4, 5 and 6.

```
col.  5   10   15   20   25   30   35   40   45   50   55   60   65
    003   A1   S1   A2   S2   A3   S3   A4   S4   A5   S5   A6   S6
```

(4) #004 Distance between atoms 1 and 2 less than between atoms 3 and 4.

```
col.  5   10   15   20   25   30   35   40   45   50   55   60   65
    004   A1   S1   A2   S2   A3   S3   A4   S4
```

(5) #005 Angle defined by atoms 1, 2 and 3 less that defined by atoms 4, 5 and 6. Atoms 2 and 5 are vertices.

```
col.  5   10   15   20   25   30   35   40   45   50   55   60   65
    005   A1   S1   A2   S2   A3   S3   A4   S4   A5   S5   A6   S6
```

(6) #006 SUM OF N ANGLES EACH DEFINED BY THREE ATOMS.

```
col.  5   10   15   20   25   30   35   40   45   50   55   60   65   70
    006    N   A1   S1   A2   S2   A3   S3   A4   S4   A5   S5   A6    1

col.  5   10   15   20   25   30   35   40   45   50   55   60   65   70
     S6   A7   S7  etc.
```

(7) #007 RMS component of thermal displacement of atoms 1 along its principal axis R (R = 1, 2 or 3).

```
col.  5   10   15   20   25   30   35   40   45   50   55   60   65   70
    007   A1   S1    R
```

#107 RMS components of thermal displacement of atoms 1 along its three principal axes.

```
col.  5   10   15
    107   A1   S1
```

#207 RMS components of thermal displacement of all NA atoms, each along its three principal axes.

```
col.  5   10   15
    207   NA   S1
```

(8) #008 Angle between principal axis R of atom 1 and a vector from atoms A2 and A3.

```
col.  5   10   15   20   25   30   35   40
    008   A1   S1    R   A2   S2   A3   S3
```

#108 Angle between each of the three principal axes of atom A1 and a vector from atoms A2 to A3.

```
col.  5   10   15   20   25   30   35   40
    108   A1   S1    -   A2   S2   A3   S3
```

#208 Angle between each of the three principal axes of all NA atoms and a vector from atoms A2 to A3.

```
col.  5   10   15   20   25   30   35   40
    208   NA   S1    -   A2   S2   A3   S3
```

(9) #009 RMS component of thermal displacement of atom A1 along its principal axis R, projected on a vector from atoms A2 and A3.

```
col.  5   10   15   20   25   30   35   40
    009   A1   S1    R   A2   S2   A3   S3
```

#109 RMS components of thermal displacement of atom A1 along its three principal axes, each projected on a vector from atoms A2 to A3.

```
col.  5   10   15   20   25   30   35   40
    109   A1   S1    -   A2   S2   A3   S3
```

#209 RMS components of thermal displacement of all NA atoms, each along its three principal axes, each projected on a vector from atoms A2 to A3.

```
col.  5   10   15   20   25   30   35   40
    209   NA   S1    -   A2   S2   A3   S3
```

(10) #010 Angle between principal axis R of atom A1 and axis I of a Cartesian coordinate system defined atoms A2, A3, A4 and A5 such that

```
   Axis 1 //  A3 - A2
   Axis 2 //  (Axis 1) X (A5 - A4)
   Axis 3 //  (Axis 1) X (Axis 2)
```

```
col.  5   10   15   20   25   30   35   40   45   50   55   60   65
    010   A1   S1    R    I   A2   S2   A3   S3   A4   S4   A5   S5
```

#110 Angle between each of the three principal axes R of atom A1 and each of three axes I of a Cartesian coordinate system defined by atoms A2, A3, A4 and A5, as described in above (#010).

```
col.  5   10   15   20   25   30   35   40   45   50   55   60   65
    010   A1   S1   --   --   A2   S2   A3   S3   A4   S4   A5   S5
```

#210 Angle between each of the three principal axes R of all NA atoms and each of three axes I of a Cartesian coordinate system defined by atoms A2, A3, A4 and A5, as described in above (#010).

```
col.  5   10   15   20   25   30   35   40   45   50   55   60   65
     010   NA   S1   --   --   A2   S2   A3   S3   A4   S4   A5   S5
```

(11) #011 RMS components of thermal displacement of atom A1 along its principal axis R, projected on axis I of a Cartesian coordinate system defined by atoms A2, A3, A4 and A5 as described above (#010).

```
col.  5   10   15   20   25   30   35   40   45   50   55   60   65
     011   A1   S1    R    I   A2   S2   A3   S3   A4   S4   A5   S5
```

#111 RMS components of thermal displacement of atom A1 along its three principal axes R, each projected on each of three axes I of a Cartesian coordinate system defined by atoms A2, A3, A4 and A5 as described above (#010).

```
col.  5   10   15   20   25   30   35   40   45   50   55   60   65
     111   A1   S1   --   --   A2   S2   A3   S3   A4   S4   A5   S5
```

#211 RMS components of thermal displacement of all NA atoms, each along its three principal axes R and each projected on the axes I of a Cartesian coordinate system defined by atoms A2, A3, A4 and A5 as described above (#010).

```
col.  5   10   15   20   25   30   35   40   45   50   55   60   65
     211   NA   S1   --   --   A2   S2   A3   S3   A4   S4   A5   S5
```

(12) #012 RMS components of thermal displacement of Atom A1 in a direction defined by atoms A2 and A3.

```
col.  5   10   15   20   25   30   35
     012   A1   S1   A2   S2   A3   S3
```

(13) #013 RMS radial thermal displacement of atom A1.

```
col.   5   10   15
      013   A1   S1
```

(14) #014 Interatomic distance averaged over thermal motion. Atom A2 is assumed to ride on atom A1.

```
col.   5   10   15   20   25
      014   A1   S1   A2   S2
```

(15) #105 Interatomic distance averaged over thermal motion. Atoms A1 and A2 are assumed to move independently.